



# INCITE awards at ALCF

Based on their potential for breakthroughs in science and engineering research, 29 of these projects have been awarded 732 million hours of computing time at Argonne's Leadership Computing Facility (ALCF) as part of the DOE's INCITE program.

The ALCF is home to DOE's Intrepid, a 40-rack IBM Blue Gene/P capable of a peak-performance of 557 Teraflops (557 trillion calculations per second). Intrepid features a low-power system-on-a-chip architecture, reducing power demands and lowering operating costs by using one-third as much electricity as other machines of comparable size.

As part of the INCITE program, the ALCF provides in-depth expertise and assistance in using ALCF systems and optimizing applications to help researchers from all different scientific disciplines to scale successfully to an unprecedented number of processors to solve some of our nation's most pressing technology challenges. This year's projects include:

## Biological Sciences

### Multiscale Blood Flow Simulations

Principal Investigator: George Karniadakis, Brown University  
Intrepid Allocation: 50,000,000 Hours

### Protein-Ligand Interaction Simulations and Analysis

Principal Investigator: T. Andrew Binkowski, Argonne National Laboratory  
Intrepid Allocation: 20,000,000 Hours

### Simulation and Modeling of Membranes Interactions with Unstructured Proteins and Computational Design of Membrane Channels for Absorption of Specified Ions

Principal Investigator: Igor Tsigelny, University of California--San Diego  
Intrepid Allocation: 4,000,000 Hours

## Chemistry

### Towards Breakthroughs in Protein Structure Calculation and Design

Principal Investigator: David Baker, University of Washington  
Intrepid Allocation: 30,000,000 Hours

### Simulations of Deflagration-to-Detonation Transition in Reactive Gases

Principal Investigator: Alexei Khokhlov, University of Chicago  
Intrepid Allocation: 18,000,000 Hours

### Potential Energy Surfaces for Simulating Complex Chemical Processes

Principal Investigator: Donald Truhlar, University of Minnesota  
Intrepid Allocation: 15,000,000 Hours

### Large Eddy Simulation of Two-phase Flow Combustion in Gas Turbines

Principal Investigator: Thierry Poinot, European Center for Research and Advanced Training in Scientific Computation  
Intrepid Allocation: 10,000,000 Hours

### Ab Initio Dynamical Simulations for the Prediction of Bulk Properties

Principal Investigator: Theresa Windus, Iowa State University  
Intrepid Allocation: 10,000,000 Hours

## Computer Science

### Performance Evaluation and Analysis Consortium End Station

Principal Investigator: Patrick Worley, Oak Ridge National Laboratory  
Intrepid Allocation: 10,000,000 Hours

### **Scalable System Software for Performance and Productivity**

Principal Investigator: Ewing Lusk, Argonne National Laboratory

Intrepid Allocation: 5,000,000 Hours

### **Trace Collection for Simulation-driven Co-design of Exascale Platforms and Codes**

Principal Investigator: David Evensky, Sandia National Laboratory

Intrepid Allocation: 5,000,000 Hours

## **Earth Science**

### **Climate-Science Computational Development Team: The Climate End Station II**

Principal Investigator: Warren Washington, National Center for Atmospheric Research

Intrepid Allocation: 40,000,000 Hours

### **Numerical Study of Multiscale Coupling in Low-Aspect Ratio Rotating Stratified Turbulence**

Principal Investigator: Susan Kurien, Los Alamos National Laboratory

Intrepid Allocation: 35,000,000 Hours

### **Deterministic Simulations of Large Regional Earthquakes at Frequencies up to 4Hz**

Principal Investigator: Thomas Jordan, University of Southern California

Intrepid Allocation: 10,000,000 Hours

## **Energy Technologies**

### **Advanced Reactor Thermal Hydraulic Modeling**

Principal Investigator: Paul Fischer, Argonne National Laboratory

Intrepid Allocation: 25,000,000 Hours

### **Large Eddy Simulation for Green Energy and Propulsion Systems**

Principal Investigator: Umesh Paliath, GE Global Research

Intrepid Allocation: 20,000,000 Hours

### **Understanding the Ultimate Battery Chemistry: Rechargeable Lithium/Air**

Principal Investigator: Jack Wells, Oak Ridge National Laboratory

Intrepid Allocation: 15,000,000 Hours

## **Engineering**

### **Detached-Eddy Simulations and Noise Predictions for Tandem Cylinders**

Principal Investigator: Philippe Spalart, Boeing

Intrepid Allocation: 45,000,000 Hours

### **Simulation of High Reynolds Number Turbulent Boundary Layers**

Principal Investigator: Robert Moser, University of Texas at Austin

Intrepid Allocation: 40,000,000 Hours

### **Turbulent Multi-material Mixing in the Richtmyer-Meshkov Instability**

Principal Investigator: Sanjiva Lele, Stanford University

Intrepid Allocation: 12,000,000 Hours

Uncertainty Quantification for Turbulent Mixing

Principal Investigator: James Glimm, State University of New York, Stony Brook

Intrepid Allocation: 10,000,000 Hours

## **Materials Science**

### **Petascale Simulations of Stress Corrosion Cracking**

Principal Investigator: Priya Vashishta, University of Southern California

Intrepid Allocation: 45,000,000 Hours

### **High-Fidelity Simulation of Complex Suspension Flow for Practical Rheometry**

Principal Investigator: William George, National Institutes of Standards and Technology

Intrepid Allocation: 25,000,000 Hours

### **Probing the Non-scalable Nano Regime in Catalytic Nanoparticles with Electronic Structure Calculations**

Principal Investigator: Jeffrey Greeley, Argonne National Laboratory

Intrepid Allocation: 15,000,000 Hours

### **Vibrational Spectroscopy of Liquid Mixtures and Solid/Liquid Interfaces**

Principal Investigator: Giulia Galli, University of California--Davis

Intrepid Allocation: 15,000,000 Hours

## Physics

### **Study of Buoyancy-driven Turbulent Nuclear Burning and Validation of Type Ia Supernova Models**

Principal Investigator: Donald Lamb, The University of Chicago

Intrepid Allocation: 80,000,000 Hours

### **Lattice QCD**

Principal Investigator: Paul Mackenzie, Fermi National Accelerator Laboratory

Intrepid Allocation: 50,000,000 Hours

### **Simulations of Laser-plasma Interactions in Targets for the National Ignition Facility and Beyond**

Principal Investigator: Denise Hinkel, Lawrence Livermore National Laboratory

Intrepid Allocation: 50,000,000 Hours

### **Nuclear Structure and Nuclear Reactions**

Principal Investigator: James Vary, Iowa State University

Intrepid Allocation: 15,000,000 Hours

### **Advanced Simulations of Plasma Microturbulence at the Petascale and Beyond**

Principal Investigator: William Tang, Princeton Plasma Physics Laboratory

Intrepid Allocation: 8,000,000 Hours

This year's allocations represent the largest amount of supercomputing time ever awarded under the INCITE program, reflecting both the growing sophistication of the field of computer modeling and simulation and the rapid expansion of supercomputing capabilities at DOE National Laboratories in recent years.

The allocations were awarded on a competitive basis under the INCITE program. The program, open to all scientists, is managed by the DOE Leadership Computing Facilities at the department's Argonne and Oak Ridge National Laboratories, which host some of the world's fastest supercomputers. Over the past 30 years, the Department of Energy's (DOE) supercomputing program has played an increasingly important role in scientific research by allowing scientists to

create more accurate models of complex processes, simulate problems once thought to be impossible, and to analyze the increasing amount of data generated by experiments.

The ALCF is dedicated to large-scale computation and builds on Argonne's strengths in high-performance computing software, advanced hardware architectures and applications expertise. Argonne is also collaborating with several institutions on developing the next generation of hardware and software for supercomputers. Called "exascale computers," they will be 1000 times faster than current machines today, performing a quintillion, or a billion billion, calculations every second.

## About Argonne

Argonne National Laboratory seeks solutions to pressing national problems in science and technology. The nation's first national laboratory, Argonne conducts leading-edge basic and applied scientific research in virtually every scientific discipline. Argonne researchers work closely with researchers from hundreds of companies, universities, and federal, state and municipal agencies to help them solve their specific problems, advance America's scientific leadership and prepare the nation for a better future. With employees from more than 60 nations, Argonne is managed by UChicago Argonne, LLC for the U.S. Department of Energy's Office of Science.

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